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Critical fluid injection volumes for uncontrolled fracture ascent.

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Timothy Davis¹, Eleonora Rivalta¹, Torsten Dahm¹

⁴ ¹GFZ (GeoForschungsZentrum), Physics of Earthquakes and Volcanoes, Helmholtzstraße 6/7, Building H ⁵ 7, 14467 Potsdam. {davis,rivalta,dahm}@gfz-potsdam.de

6	Key Points:
7	• Three-dimensional threshold volumes for self-sustained fluid-filled fracture ascent
8	• We derive analytical equation and validate it through numerical boundary-element
9	simulations
10	• Assessing safe hydro-fracture operation volumes requires quantitative modeling
11	of in-situ complexities

Corresponding author: Timothy Davis, davis@gfz-potsdam.de

12 Abstract

Hydro-fracturing is a routine industrial technique whose safety depends on fractures re-13 maining confined within the target rock volume. Both observations and theoretical mod-14 els show that, if the fluid volume is larger than a critical value, pockets of fluid can prop-15 agate large distances in the Earth's crust in a self-sustained, uncontrolled manner. Ex-16 isting models for such critical volumes are unsatisfactory, most are two-dimensional and 17 depend on poorly constrained parameters (typically the fracture length). Here we de-18 rive both analytically and numerically in three dimensions scale-independent critical vol-19 umes as a function of only rock and fluid properties. We apply our model to gas, wa-20 ter and magma injections in laboratory, industrial and natural settings, showing that our 21 critical volumes are consistent with observations and can be used as conservative esti-22 mates. We discuss competing mechanisms promoting fracture arrest, whose quantita-23 tive study could help to assess more comprehensively the safety of hydro-fracturing op-24 erations. 25

²⁶ Plain Language Summary

Fractures in rocks can act as channels for fluids. Fracking, or hydro-fracturing, in-27 volves injection of fluids at high pressure in order to grow fractures within the rock and 28 increase its permeability. Fluid volumes need to be kept below a threshold value: if the 29 fluid volume is larger, then the stresses at the tips of the fluid pocket will be large enough 30 31 for the fluids force their way around by fracturing the rock ahead of them. Previous theoretical models for the critical volumes are unsatisfactory as they are two-dimensional 32 and based on poorly constrained parameters. We derive and test a new three-dimensional 33 equation that uses only rock and fluid parameters. We find that typical volumes injected 34 in hydro-fracturing operations are over the limit we define. We argue they are still mostly 35 safe as additional processes often hinder fracture growth. Further work is needed to com-36 prehensively quantify mechanisms that hinder hydro-fracture arrest. 37

38 1 Introduction

Official guidelines for hydraulic fracturing (e.g., Mair et al., 2012; EPA, 2016), outline safe operational practices for regulators. Such reports often state that during routine operations fractures are unlikely to grow out of the target rock formation, as typical injection pressures are too low for this to occur. These claims are substantiated with empirical observations from closed access microseismic data of scarce vertical fracture growth following injection (Fisher & Warpinski, 2012). Evidence for unsafe vertical migration of such fluids remains ambiguous (Vidic et al., 2013).

Natural analogues of fluid migration by hydro-fracturing include drainage crevasses 46 in melting glaciers and magma transport by dyking. Field and experimental observations 47 provide some indication of typical rates of fracture ascent, in the order of mm/s to around 48 half a m/s (Das et al., 2008; Tolstoy et al., 2006). For water-filled fractures in rock this 49 has not been observed; estimates from geochemical analysis supply similar rates of ~ 0.01 -50 0.1 m/s, (1 km/day) (Okamoto & Tsuchiya, 2009). Theoretical arguments suggest that 51 the migration velocity should have a dependency on volume (Heimpel & Olson, 1994; 52 Dahm, 2000). 53

According to theory, tip-propagation occurs when a critical amount of fluid has accumulated inducing enough stress to overcome the medium's fracture toughness, K_c (Secor & Pollard, 1975). So far, critical 'volumes' are given in terms of the fracture length, which is not directly observable and difficult to estimate from observations (Secor & Pollard, 1975; Dahm, 2000; Taisne et al., 2011); moreover, such analyses have been carried out in 2D only, not capturing the fracture's 3D shape and scaling of volume vs length.

Figure 1. A) Stress vs depth in the crust, data from Bell et al. (1990), crack shown in red with length 2*c*. B) Stress boundary conditions and 3D crack wall displacement. C) Cross sections of crack wall displacement, itp=interpenetration. D) Shape of an ascending air filled crack in gelatine from (Rivalta & Dahm, 2006). E) Air filled cracks tip-line vs a penny-shaped tip-line.



Here, after deriving a theoretical model and validating it with numerical simula tions, we apply this to cracks filled with air, water, oil and magma in solids of varying
 stiffness and toughness, across a wide range of length scales.

63 Methods

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1.1 Hydrofracturing and stress gradients

⁶⁵ We consider a pressurised penny-shaped crack of radius c and volume V in an elas-⁶⁶ tic medium. The crack can only grow when the stress intensity K_I at its tip-line exceeds ⁶⁷ K_c . The elastic parameters of the medium (shear modulus, μ , and Poisson's ratio, ν) con-⁶⁸ trol the fracture's aperture. The internal pressure p_0 must overcome the stress normal ⁶⁹ to the crack walls (generally the minimum compressive stress, σ_{min}) by an amount ac-⁷⁰ commodating the volume V against the elastic forces, Fig. 1A/B.

When the crack is vertical, the gradient in the normal stress acting to close the crack 71 and the gradient in the load due to the overlying fluid acting to open the crack, i.e. $\rho_r g$ 72 and $\rho_f g$ in Fig. 1A, where ρ_r and ρ_f are the densities of the host rock and fluid, respec-73 tively, result in a net stress gradient $\Delta \gamma$ acting to push open the crack walls in an in-74 verse 'teardrop' shape, Fig. 1B/C. When the crack is inclined $\Delta\gamma$ needs to be adjusted 75 by $\cos(\theta)$, where θ is the cracks' angle away from vertical. Quantitative formulations used 76 to assess industrial fracture heights neglect stress gradients (e.g., Xu et al., 2019; Yue 77 et al., 2019). This contrasts with routine observations of stress gradients from industry 78

⁷⁹ data (Fig. 1A) and the fact that these gradients are considered in the well design of in-

dustrial operations (Lecampion et al., 2013; Mair et al., 2012). When this gradient is in-

cluded in formulations, stress intensity varies around the fracture's tip-line (Fig. 2). Where K_c is exceeded, the upper tip-line advances. The contained fluid flows into this newly

 K_c is exceeded, the upper tip-line advances. The contained fluid flows into this newly created fracture surface while the bottom edge of the fracture is pinched shut as the in-

ternal pressure drops. With a great enough volume this fluid movement maintains a crit-

ically stressed upper tip-line and the fracture reaches a state of 'self-sustaining propa-

gation'. Fluid viscosity will cause some fluid to stay trapped in the tail trailing behind

the fracture; if fluid viscosity is low enough, the contained fluid is virtually all transported.

Provided the fracture's shape and volume are maintained, no additional forces, such as

⁸⁹ pressure from injection, are required to aid this state of propagation.

1.2 Analytical formulation

Secon and Pollard (1975) define in 2D the size and pressure inside a vertical fracture subject to $\Delta \gamma = (\rho_r - \rho_f)g$ such that at the upper tip $K_I^+ = K_c$ and at the lower tip $K_I^- = 0$. We derive an analytical expression for the fluid volume needed for a threedimensional crack to propagate in a self-sustained manner.

 K_I for a mode I penny-shaped fracture of radius c subject to a generic linear stress gradient can be expressed as the superposition of K_I for a penny-shaped fracture subject to a uniform pressure p_0 :

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$$K_I = \frac{2}{\pi} p_0 \sqrt{\pi c} \tag{1}$$

⁹⁹ and that for a penny-shaped fracture subject to a linear pressure gradient $\Delta \gamma$ where pres-¹⁰⁰ sure is equal to 0 at the fracture's midpoint (Tada et al., 2000, p. 355):

$$K_I^{\pm} = \pm \frac{4}{3\pi} \Delta \gamma c \sqrt{\pi c} \tag{2}$$

where the + refers to the propagating tip and the - to the basal tip. Requiring $K_I^- = 0$ results in $p_0 = 2\Delta\gamma c/3$ and thus:

$$p^{\pm} = \left(\frac{2}{3} \pm 1\right) \Delta \gamma c \tag{3}$$

Requiring $K_I^+ = K_c$ and rearranging for c yields:

$$c = \left(\frac{3\sqrt{\pi}K_c}{8\Delta\gamma}\right)^{2/3}\tag{4}$$

We note that the 2D plane strain critical length is $\approx 0.9c$. The volume of the crack can be calculated based on the equation for a crack pressurised by uniform pressure p_0 , as the antisymmetric pressure contribution integrates to zero. Thus using (Tada et al., 2000):

$$V = \frac{8(1-\nu)}{3\mu} p_0 c^3 \tag{5}$$

¹¹¹ results in:

$$V_{c}^{an} = \frac{(1-\nu)}{16\mu} \left(\frac{9\pi^{4}K_{c}^{8}}{\cos(\theta)\Delta\gamma^{5}}\right)^{1/3}$$
(6)

This equation requires validation in order to evaluate the bias due to approximating the shape of the propagating crack as circular (Fig. 1D/E).

1.3 Numerical model

To simulate propagation, we use a 3D Boundary Element program where each element is a triangular dislocation with constant displacement (Fig. 2) (Nikkhoo & Walter, 2015). The program computes fracture opening and stress intensities, based on fracture shape, rock and fluid parameters and external stresses Davis et al. (2019). Our workflow during each iteration is as follows:

Figure 2. Numerical simulation of crack propagation (from left to right), looking at the fractures' face (left) and cross section (right). Grey points are edges that closed in the previous iteration.



121	1. We invert for the uniform internal fluid pressure, p_0 , necessary to open the crack
122	to match the required volume against all external and internal tractions. Non-linear
123	complementarity conditions are imposed such that the crack's faces cannot inter-
124	penetrate (Davis et al., 2019).
125	2. We calculate the crack opening and the stress intensity at the tipline using the method
126	of Davis et al. (2019). In order to reduce artefacts, we smooth the stress inten-
127	sity along the tip line by averaging the local K_I with its two neighbouring edges.
128	3. We calculate the advance or retreat of the tipline. At elements where K_I exceeds
129	K_c , the tip-line will advance proportional to K_I/K_c . This approximation is akin
130	to the "Paris fatigue law" (Lecampion et al., 2018). The maximum crack advance
131	will occur at the triangle where K_I is maximum; this advance is set equal to the
132	mesh's average triangle size. The triangular elements that close are removed. The
133	simulation assumes the fluid is inviscid, and, as such, we cannot retrieve time-dependent
134	propagation rates.
135	4. Once the fracture's edge has been updated, it is re-meshed and cleaned such that
136	the triangles on the fractures tip-line are approximately equal size and isosceles
137	(Da & Cohen-Steiner, 2019).

For a description of the numerical methods accuracy, see the appendix. We start the simulation with a vertical penny-shaped crack. We fix the number of elements, K_c , $\Delta\gamma$, μ , ν and the volume of fluid, V. We set the initial radius to 0.4c, (Eq. 4). In our 350+ simulations we use variables spanning several orders of magnitude: G=190-5·10¹⁰Pa, $\nu=0.25-0.49$, $\Delta\gamma=7.8\cdot10^2-2.2\cdot10^4$ Pa·m⁻¹ and $K_c=1-1\cdot10^8$ Pa·m^{0.5}. We state the fracture has reached self-sustaining ascent when its upper tip has travelled 4c upwards.

For all simulations, independent of mesh sampling, we find that if $V = 0.7V_c^{an}$ the numerical code returns a trapped fracture and if $V = 0.8V_c^{an}$ the fracture always reaches self-sustaining propagation. Therefore, scaling Eq. 6 by 0.75 supplies the numerical estimate of V_c , independent of the scale we use:

$$V_c^{num} = 0.75 \frac{(1-\nu)}{16\mu} \left(\frac{9\pi^4 K_c^8}{\cos(\theta)\Delta\gamma^5}\right)^{1/3}$$
(7)

For all cracks that reached self-sustaining propagation the horizontal and vertical lengths were greater than $\sim 0.6c$ and $\sim 1.14c$, respectively. **Figure 3.** $V^*\mu$ vs K_c from Heimpel and Olson (1994). Eq. 7 predictions shown as black lines. The thickness of the grey filled patches represents the velocity of the crack as the volume increases, normalised by maximum observed velocity.



151 **2** Applications

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2.1 Analog gelatine experiments

The analog study of Heimpel and Olson (1994) inspects critical volumes of fluids 153 ascending in gelatine blocks of different stiffness and fracture toughness (Fig. 3). The 154 graph of volume vs speed from their experimental results shows a rapid increase in speed 155 past a certain volume. The authors interpret that at velocities past $\sim 0.7 \ cm/s$ (crosses 156 in Fig. 3), the ascent transitions from a sub-critical propagation regime $(K_I < K_c)$; where 157 the fracture growth speed at the tip limits the velocity (Atkinson & Meredith, 1987), to 158 a dynamic propagation regime. We test if our equation can predict volume of fluid that 159 causes this transition in ascent speed. As Heimpel and Olson (1994) estimate K_c directly 160 from this change in velocity, to verify that we can use this estimation, we calculate K_c 161 differently; directly from the measured value of G. Strain energy release \mathcal{G} increases with 162 greater stiffness in gelatin solids: $\mathcal{G}[N/m] \approx 6.66 \cdot 10^{-4} G[Pa]$ (Czerner et al., 2016). This 163

¹⁶⁴ second independent estimate of K_c lies within 5 Pa·m^{1/2} of the original estimate. Us-¹⁶⁵ ing $\rho_r = 1000 \text{ kg} \cdot \text{m}^{-3}$, $\nu = 0.5$ and setting μ , ρ_f and K_c to match the experiments of Heimpel ¹⁶⁶ and Olson (1994), we find that our value of V_c^{num} independently captures the point at ¹⁶⁷ which the velocity transitions, described above, supporting the previous interpretation ¹⁶⁸ that this describes the transition to dynamic fracture propagation.

2.2 Magmatic dykes

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We consider magma propagation volumes at Piton de la Fournaise, La Réunion, 170 to see how our equation matches observed dyke volumes. The volumes of the dyke in-171 trusions observed between 1998-2016 range from $0.05 \cdot 3.2 \cdot 10^6 \cdot m^3$ (Froger et al., 2004; Fukushima 172 et al., 2005, 2010; Smittarello et al., 2019). Using $\rho_r - \rho_f = 100 \text{ kg} \cdot \text{m}^{-3}$, $\mu = 5 \text{ GPa}$, $\nu = 0.25$ 173 and K_c ranging from 29 to 112 MPa·m^{1/2} (Fukushima et al., 2010; Delaney & Pollard, 174 1981), we retrieve $V_c^{num} = 0.05 \cdot 10^6$ and $2 \cdot 10^6 \cdot \text{m}^3$, respectively. The critical volumes we 175 estimate are consistent with the observed dyke sizes. As such our approximation pre-176 dicts the correct scale in natural settings, provided K_c values estimated from field data 177 are used, noting such field values appear to correct due to a number of additional pro-178 cesses that we have disregarded, instead of being representative of the rock strength at 179 the scale of a laboratory sample. 180

2.3 Water injection into stiff rock

The UK government defines hydraulic fracturing as operations that use over 1,000 182 m^3 of fluid per frack stage. During a hydro-fracturing procedure, proppant is injected 183 in the final phase to maintain an open fracture (e.g. spherical quartz grains). After the 184 operation, not all injected fluid is recovered when the wellhead valve is opened: Vidic 185 et al. (2013) report an average of only 10% fluid recovery in flowback waters, noting that 186 this recovery volume decreases when shut-in times are longer. Using $\rho_r = 2700 \text{ kg} \cdot \text{m}^{-3}$ 187 $\rho_f = 1000 \text{ kg} \cdot \text{m}^{-3}$, $\mu = 8.9 \text{ GPa}$, $\nu = 0.25 \text{ and } K_c$ in the range 0.36–4.05 to 7–25 MPa·m^{1/2}, we obtain $V_c^{num} = 6 \cdot 10^{-2}$ and 500 m³ respectively. These K_c values are for laboratory-188 189 sized shale samples from 100 to 1000 m confining pressure and effective K_c values esti-190 mated for veins in the field, respectively (Gehne et al., 2020; Olson, 2003). Current op-191 erations use volumes around double our highest predicted limit. Few observations at-192 test to the fact that industrial operations can cause ascent of fluids in fractures. One such 193 example, are the spectacular surface fissures created due to steam injection documented in Schultz (2016); additional examples can be found in Schultz et al. (2016). Geochem-195 ical data from aquifers above fracking operation sites has shown some evidence of the 196 contamination of overlying units, which is attributed to poor well casing design, rather 197 than fracture ascent (Vidic et al., 2013). Usually, microseismic monitoring of actual frack-198 ing operations show limited vertical extents of the fractures, however, these data are pro-199 prietary and methodological descriptions are scarce (Fisher & Warpinski, 2012). Exper-200 imental fracturing data is of little help as volumes injected are typically below or close 201 to our volumetric limit, with injected volumes of 2 to 20 m³ (Warpinski et al., 1982; Pan-202 durangan et al., 2016). 203

Natural degassing, such as CO_2 in the Cheb basin, Czech Republic, has chemical 204 signatures of fluids that have ascended over 20 km through the crust (Weinlich, 2014). 205 Fracture driven ascent can explain this phenomena without the requirement of permanent highly conductive fluid pathways at great depths. Supercritical CO_2 at depth has 207 a similar density to water, and as such may be a good natural analog for water filled frac-208 ture ascent. We saw that in analogue and magmatic examples Eq. 7 predicts the cor-209 210 rect order of magnitude of critical volumes; at the same time, it appears that this equation is conservative for high volume water injection as fracture ascent in these settings 211 has rarely been observed. 212



Figure 4. Processes that can hinder fracture ascent, K and V relate to effective K_c and V_c operating in Eq. 7

3 Discussion and conclusions

In summary, Eq. 7 provides an estimate of the minimum fluid volume for self-sustained 214 propagation of fluid-filled fractures, ranging from cm to tens of km. V_c is dependent on 215 $K_c^{8/3}$; since K_c is often poorly constrained V_c suffers from large uncertainties. Values of 216 K_c obtained in laboratory experiments show a strong dependency on pressure and tem-217 perature. Field estimates of effective K_c from trapped fractures can be orders of mag-218 nitude larger. An effective way to estimate K_c in Eq. 7 incorporating all processes af-219 fecting the energy needed to extend the fracture at different scales would clearly be ben-220 eficial for any fracture mechanics based analysis of rock masses and the resultant inter-221 pretations. 222

In our derivation we have neglected the effects of viscosity. Whether these effects 223 will dominate over toughness in determining fracture growth can be assessed by eval-224 uating the time scale needed for the fluid pressure to equilibrate within the crack, as this 225 will mean that viscous dissipation is low and crack growth will be toughness-dominated 226 (Bunger & Detournay, 2007). The model of Bunger and Detournay (2007) assumes a con-227 stant injection rate with no stress gradients, we assume this still provides a rough esti-228 mate of the timescale until this transition. Typical industrial operations use fluid vis-229 cosity of 0.001-0.01 Pa·s, injection rates between 0.5-10 m³/min and stiffness's of 10-40 230 GPa. Using low values of K_c from laboratory experiments in shale, 0.36 MPa m^{1/2}, this 231 transition time ranges between 1 minute to times exceeding the end of injection. Whereas, 232 setting K_c higher, values for shale at depth, e.g. 4 MPa·m^{1/2} this significantly reduces 233 this range from milliseconds to a maximum of 5 hours. This suggests that, depending 234 on K_c , Eq. 7 can be a relevant estimate of V_c^{num} , independent of viscous forces. 235

While theory and experiments support Eq. 7, this appears to be overly conservative in practice, as injections of quantities of fluid exceeding this do not result in significant ascent in most cases. In part, this discrepancy results from our simplification of the process, as mass conserving propagation in a homogeneous linear-elastic medium.

- Fig. 4 shows a schematic of processes not quantified in relation to critical fluid volumes which we review in detail below.
- 1. A series of mechanisms can reduce V during propagation and thus promote crack 242 arrest. These include leak-off from the fractures faces, the fracture becoming mul-243 tistranded/compartmentalised, fluid recovery (extraction), or fluid remaining in 244 the tail of the fracture due to added proppant or viscous forces (Taisne & Tait, 245 2009).246 2. Mechanisms that can lead to an effective increase of K_c , and thus also promote 247 crack arrest, include plastic tip processes, the fracture entering in a zone of dam-248 age of the host rock (Sih et al., 1965; Kaya & Erdogan, 1980), or seismicity sur-249 rounding the fracture, causing reduction in the system's energy/blunting the frac-250 ture's tip (Rivalta et al., 2015). 251 3. Heterogeneous μ or K_c or stress barriers may also lead to arrest of fractures by 252 deflection or promoting lateral growth (Maccaferri et al., 2011; Bunger & Lecam-253 pion, 2017; Warpinski et al., 1985), 254 4. Eq. 7 has a clear dependency on the fracture's dip. If the minimum compressive 255
 - 4. Eq. 7 has a clear dependency on the fracture's dip. If the minimum compressive stress is vertical, this promotes flat lying fractures.

Quantification of processes acting to halt fracture ascent, especially in the context of the variables in our equation, are critical to understand which volumetric limits can be deemed safe. In particular, the gradient in stress with depth must be included to assess this process. Without such quantification, regulation of this industrial process will continue to rely on empirical evidence for safe rates, volumes and depths from select operations that may not be representative.

²⁶³ Appendix A Numerical

A1 Numerical accuracy

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We verify that our method to compute K_I is independent of crack shape and bound-265 ary condition. Previously this was only compared to solutions for a circular crack sub-266 ject to uniform stresses (Davis et al., 2019). We compare this to the analytical solution 267 for the stress intensity around an elliptical crack, subject to a superposition of uniform 268 pressure and a linear gradient of stress, such that, at the basal tip, $K_I = 0$ (Fig. 1) (Atroshchenko 269 et al., 2009). We note that under a stress gradient, K_I for vertically aligned elliptical 270 cracks is not maximal at its upper tip, due to the reduction in crack surface area prox-271 imal to this edge. 272

For a mesh with 650 triangles (Fig. A1A/B), the greatest vertical separation between the numerical points and the analytical line is 0.09. For this test we required the edge points of the mesh's triangles, not the midpoints of the triangles edge where K_I is calculated, to lie on the tip-line defined by the analytical solution. For a mesh with 1500 triangles (Fig. A1C/D), the maximum vertical distance from the analytical solution of is 0.06, noting that greater sampling does not necessarily converge to a improved accuracy, see appendix of Davis et al. (2019).

As a further test of numerical accuracy, we compare how well the numerical method approximates the opening volume of a penny shaped crack subject to tension (Tada et al., 2000). We find a sampling of 650 triangles overestimates the volume by 5.2%, by increasing the triangle count to 1500 this drops to 3.5%.

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Figure A1. Stress intensity factor approximation using the 3D displacement discontinuity method. A/C) Elliptical crack meshed with 650/1500 triangles respectively, B/D) Numerical (dots) and analytical (solid line) results. Results are normalised relative to the maximum analytical value of K_I .

